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NMR and calorimetry of CuAgSe and $CuAgSe_{0.5}Te_{0.5}$[1] EMILY CONANT, ALI SIRUSI, Texas AM University, SEDAT BALLIKAYA, University of Michigan, Istanbul University , KESHAB DAHAL, ZHIFENG REN, University of Houston , CITRAD UHER, University of Michigan, JOSEPH ROSS, Texas AM University — Copper based chalcogenides have attracted much interest due to potential electronic and thermoelectric applications, and CuAgSe in particular has been found to have very low thermal conductivity and high mobility, with the possibility of Dirac-like electronic features. We have used ^{63}Cu, ^{65}Cu, and ^{77}Se NMR along with specific heat and DFT computation to study the structure, vibrational and electronic properties. We observe a large Einstein-like mode in the CuAgSe specific heat, which we discuss in terms of Cu hopping between half-occupied sites. DFT energy minimization and computed phonon behavior also support this result. The Cu NMR T_1^{-1} is dominated by phonons at low temperatures, also indicative of strongly anharmonic vibrational behavior, which may contribute to the lower thermal conductivity. At higher temperatures, Se NMR shows evidence for Cu hopping. We also examined Cu NMR shifts and find that the metallic shift makes up a very small portion, however based on the reported effective mass the results indicate that Cu s states make a significant contribution to the conduction band, contrary to computational results.

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